

# Gold Thermocompression Wafer Bonding

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**Abstract**—Thermocompression bonding of gold is a promising technique for the fabrication and packaging microelectronic and MEMS devices. The use of a gold interlayer and moderate temperatures and pressures results in a hermetic, electrically conductive bond. This paper documents work conducted to model the effect of patterning in causing pressure non-uniformities across the wafer and its effect on the subsequent fracture response. A finite element model was created that revealed pattern-dependent local pressure variations of more than a factor of three. This variation is consistent with experimental observations of bond quality across individual wafers. A cohesive zone model was used to investigate the resulting effect of non-uniform bond quality on the fracture behavior. A good, qualitative agreement was obtained with experimental observations of the load-displacement response of bonds in fracture tests.

**Index Terms**—wafer bonding, thermocompression, cohesive zone.

## I. INTRODUCTION

WAFER bonding is emerging as a key technology for microelectronic devices and microelectromechanical systems (MEMS) [1-4]. The ability to create three-dimensional structures, such as 3-D interconnects for microelectronics or capped fluid channels for MEMS is very important. In addition wafer bonding is being viewed as an important process for packaging of both MEMS and microelectronics. The ability to perform these operations at the wafer-level, operating on many devices in parallel, has large economic benefits. In addition, the ability to encapsulate devices before die-sawing is beneficial as it will protect the devices from the particles and fluids associated with die-sawing.

Several wafer bonding technologies exist, that offer complementary features. Gold thermocompression bonding has the particular attributes of providing a conductive bond, and requiring relatively low temperatures and pressures to create it. In addition the bond is hermetic and the use of a metal interlayer potentially makes the bond less sensitive to surface roughness and other flatness variations. Thermocompression bonding has been widely used for creating interconnects to first level packaging for chip

input/output [5,6], however, relatively little work has been conducted to examine the feasibility of wafer-level bonding. Key questions revolve around the sensitivity of the bond to wafer flatness variations, pressure variations, and patterning. In addition the tooling used to perform wafer level thermocompression bonding has not been optimized for the demands of this particular bonding method.

Previous work conducted by the present authors revealed that considerable variation in the appearance of bond fracture surfaces and irregularity in the load-displacement response of fracture tests [7-9]. The work presented in this paper aims to provide simulation results to verify the role of patterning in creating the observed non-uniform bonds and to confirm that variations in bond toughness and strength are consistent with the observed non-idealities in the force-displacement behavior observed during fracture tests.

The paper is structured as follows. Section II provides a short overview of the wafer-level thermocompression process and the mechanical testing used to characterize it. Section III documents the finite element analysis and results used to investigate the contribution of patterning to pressure non-uniformity across the wafer. Section IV presents a cohesive zone model and results used to investigate the role of bond-quality variations across the wafer on the force displacement response. Section V discusses the results and section VI provides a summary and conclusions.

## II. EXPERIMENTAL APPROACH

In the current work pairs of wafers were coated with 0.2-1  $\mu\text{m}$  of gold on each wafer. A silicon oxide diffusion barrier and titanium adhesion layer were utilized, based on the results of earlier work. The gold was patterned using a lift-off mask technique. The basic pattern used in the current work consisted of sets of parallel gold lines, 50  $\mu\text{m}$  wide, with the pattern on one wafer rotated through 90° relative to the other to give discrete bonding locations at the cross-over points, as shown in figure 1. This pattern replicates that envisioned for practical applications; consisting of seal rings, or bond pads for through-thickness electrical connections. In addition the use of these patterns increases the pressure applied to an individual contact point during bonding, and also reduces the load required to cause fracture of the pair of bonded wafers during testing. Both of these effects make the experimental procedures easier to perform.

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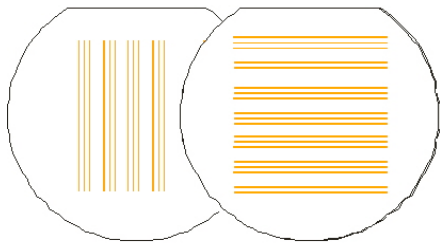


Fig. 1. Schematic of line patterns on pairs of wafers

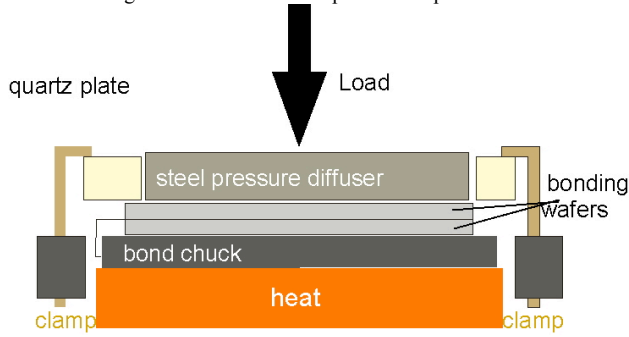


Fig. 2. Schematic of bonding apparatus

The pair of wafers were then inserted into a commercial aligner-bonded and subjected to temperatures in the range 250-350 °C and pressures applied to the wafer in the range 0.2-1 MPa. This is shown schematically in figure 2. The bonded wafer pairs were then die-sawed into four point bend delamination mechanical test specimens. These specimens were then loaded in four point bending until bond fracture had occurred. Figure 3 shows the load displacement curve for an ideal bond fracture in which the bond propagates at constant load, corresponding to constant toughness.

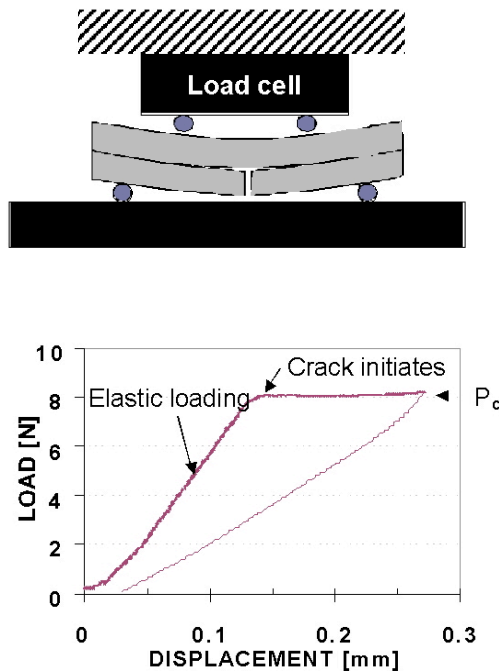


Fig. 3. Schematic of four point bend delamination apparatus and an ideal load displacement curve.

In many cases bond fracture did not occur at constant load, and two more typical load-displacement curves are shown in figure 4. In these cases the load displacement response does not have a sharp transition from the initial linear-elastic loading to the crack propagation phase. In addition there are several load drops during the crack propagation phase, which indicate discontinuous crack-propagation and arrest. This was confirmed by *in situ* observations of the crack propagation using a long working distance microscope during mechanical testing.

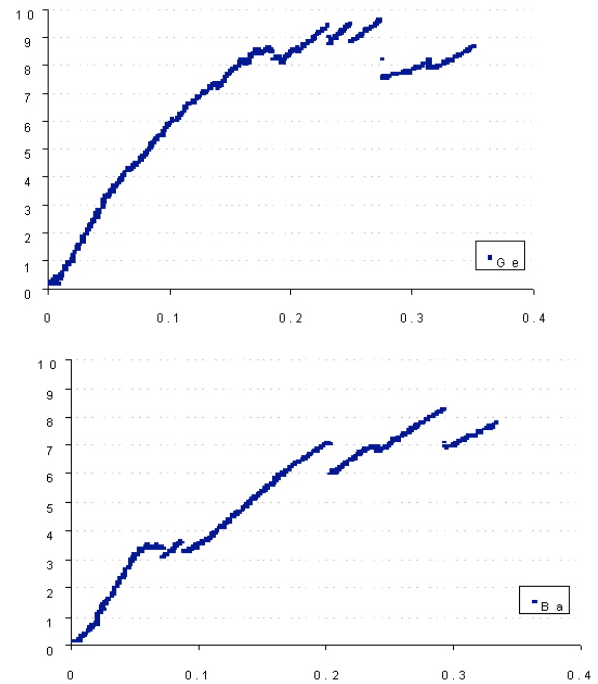


Fig. 4. Two non-ideal load displacement curves from four-point bend delamination tests.

Microscopic examination of the fracture surfaces revealed wide variation in the degree of ductility demonstrated in the gold bond pads, ranging from very little ductility, to plastic strains approaching unity. This variation could occur between neighbouring pads and occurred within individual test specimens and across wafers. Atomic force microscope images of two fracture surfaces are shown in figure 5.

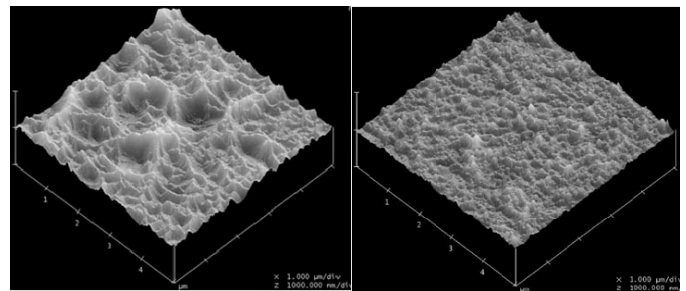


Fig. 5. Two AFM images showing the variation in ductility from fracture surfaces. In the left hand image the RMS roughness is 82 nm, and on the right only 36 nm.

Given these observations it seemed likely that the variation in fracture behavior across individual test specimens, and across wafers was likely to be due to local variations in the pressure applied to the gold layers. The variation in load-displacement response in the fracture tests could then be ascribed to the variations in bond toughness across the wafer. Models were constructed to investigate these factors.

### III PRESSURE UNIFORMITY MODEL

Several factors could contribute to non-uniformity of the applied pressure on the gold. Gold thickness variations, tooling and wafer flatness variations, tool misalignment, temperature variations and gold property variations are all possibilities. All of these were considered and rejected as being the likely primary cause of the experimentally observed variations in bond fracture appearance. It was felt that the most likely source of variation was due to the patterning of the gold.

A finite element model was constructed so as to be representative of the typical bonding configuration. Arrays of gold bond pads were assigned elastic-plastic properties of the gold. The bond pads were arranged in groups of eleven evenly spaced pads with wider gaps between groups pads. The wafers were modeled explicitly as elastic structures with the properties of silicon. The models were loaded with varying boundary conditions, to bound the experimentally applied conditions. Symmetry was assumed so that only one set of bond pads were modeled as shown in figure 6.

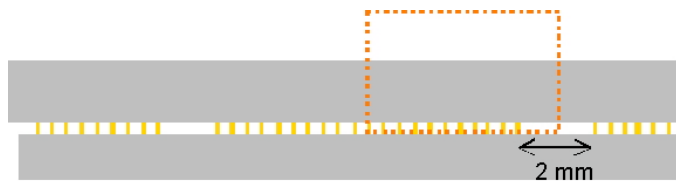


Fig. 6. Bond-pad configuration modeled.

The model was implemented using the ABAQUS commercial finite element software. A course mesh was used for most of the silicon wafers. A refined mesh was used for the bond pad regions, with five elements through the thickness of the pads, and ten elements across their width. The mesh is shown in figure 7.

A set of model results are shown in figure 8. The model predicts a uniform pressure over the inner seven pads, but then an increasing pressure towards the edge. The pressure applied to the pad at the edge of the group was three to five times higher than the pressure applied at the center of the group of bond pads. Study of the effect of the steel diffuser plate (see figure 2) indicated that for a uniform pressure loading the diffuser plate was redundant, however, it played a key role in compensating for the inadvertent application of a point load. It seems likely that the patterning of the gold is the major contribution to the variations in applied pressure and resulting variations in bond quality observed experimentally.

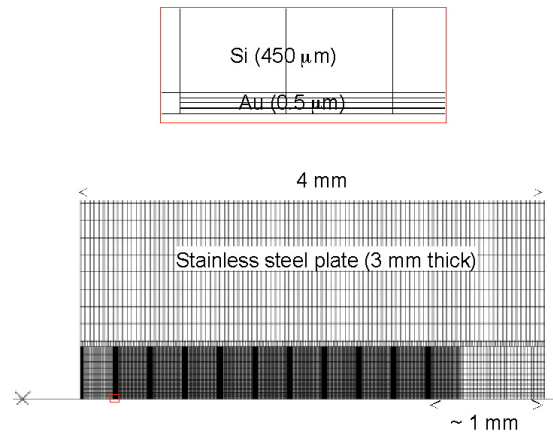


Fig. 7. Finite element mesh of bonding model.

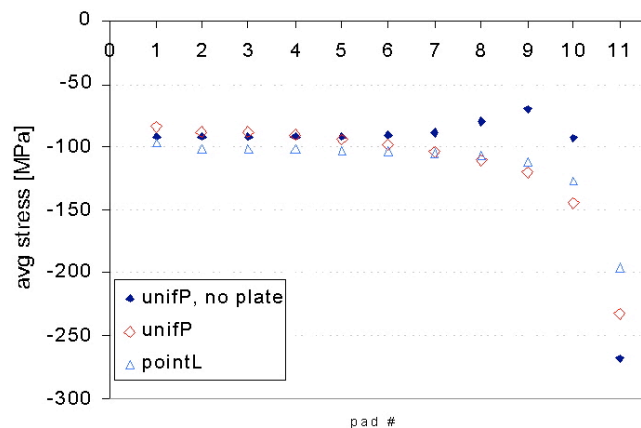


Fig. 8. Pressure distribution as a function of bond pad location. Pads 10 and 11 carry the highest local pressure. The three sets of results correspond to three loading cases in figure 2: Uniform pressure, no diffuser plate, uniform pressure, and a point load.

The analysis presented here utilized a two dimensional, plane-strain representation of the bond case. A full three dimensional finite element model was constructed to verify that the results of the 2-D model corresponded to the reality of the experiments. Very similar variations in local pressure were observed in the three-dimensional case, providing validation of the two dimensional results.

Experimental observations revealed similar behavior in experiments. In wafer pairs with variable bond quality, the well bonded pads would tend to be around the edges of the groups of lines, as shown in figure 9. It is also worth noting that there was considerable additional variation in the experimental observations of well and poorly bonded pads.

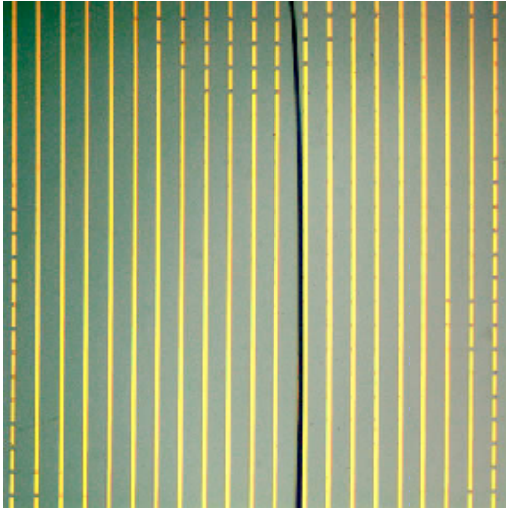


Fig. 9. Optical micrograph showing the fracture surface of a thermocompression bonded fracture specimen. The well bonded pads appear dark and are clustered around the edge of the group of lines.

#### IV COHESIVE ZONE MODEL

Given the variation in pressure, it is likely that a variation in bond quality results. In order to investigate the effect of such a variation in bond-quality on the resulting bond integrity, a cohesive zone model was used. This assigns a load-displacement response to the material of an individual bond, or fraction of a bond pad. A typical cohesive behavior is shown in figure 10.

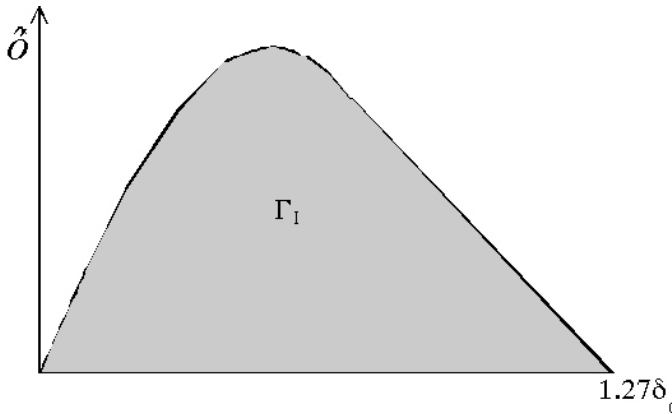


Fig. 10. Cohesive model used to represent the stress-displacement of the gold bond pads during fracture testing.

The key parameters of the model are the stress,  $\sigma$ , displacement,  $\delta$  and the area under the curve, which corresponds to the toughness,  $\Gamma$ . A higher value of  $\Gamma$  corresponds to a higher quality bond. The results of the model are relative insensitive to the shape of the cohesive model, and for the present work a rounded shape was chosen as this improved the numerical stability of the results. This was modified from earlier work by Yang and Thouless [10]. They utilized a trapezoidal cohesive model with an elastic ramp up to a maximum stress plateau and a linear ramp down to the maximum displacement point. The vertices in the Yang and Thouless model caused problems with convergence

for the discontinuous bonds used in the present work.

No attempt was made to measure the cohesive response of individual gold pads directly, and the results of this model should be regarded as providing qualitative insight as to the experimental observations. The cohesive model was implemented as a user-defined material model in the ABAQUS finite element software. Three problem types were simulated. Continuous bonds, discontinuous bonds with uniform period, and discontinuous bonds of uneven period, as tested in the experimental work. These configurations are shown schematically in figure 11.

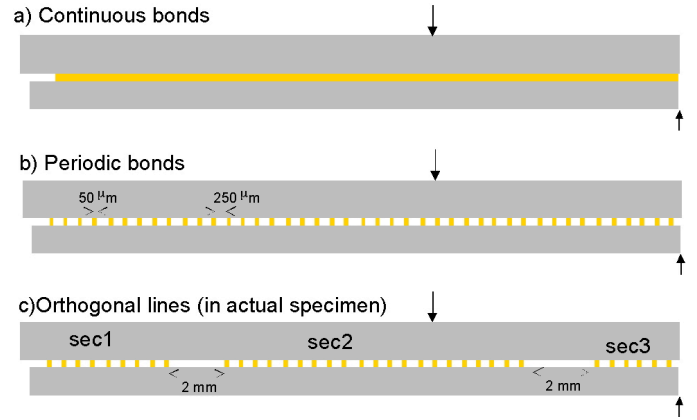


Fig. 11. Three problem categories modeled using the cohesive zone model.

The results of the continuous and uniform periodic bonds demonstrated load-displacement behavior corresponding closely to the “ideal” behavior of crack propagation at constant load shown in figure 3. The toughness observed macroscopically, by calculating from the load at which crack propagation occurred, corresponded to the toughness of the cohesive zone model. These simulation results are shown in figures 12 and 13.

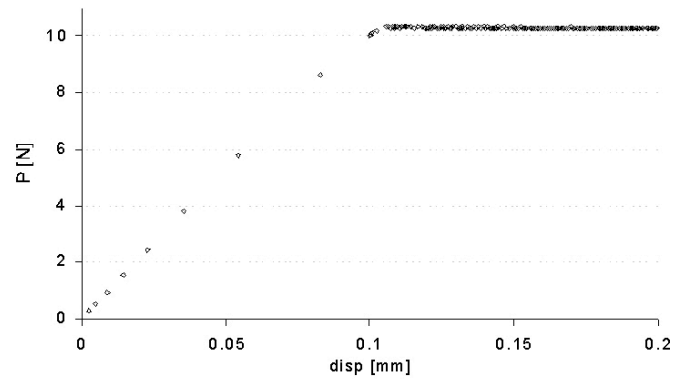


Fig. 12. Simulated load displacement response for a continuous bond, with uniform bond toughness.

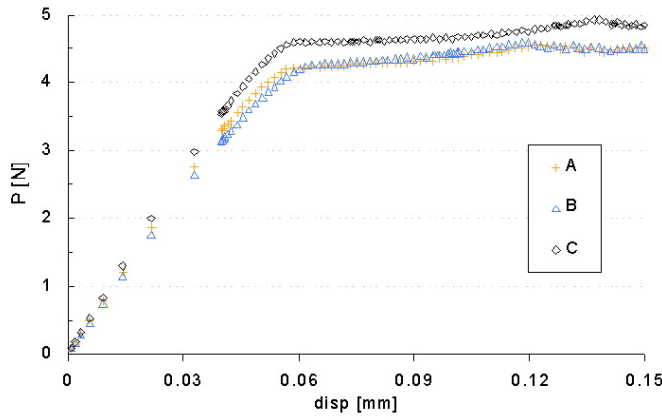


Fig. 13. Simulated load displacement response for a discontinuous bond, with uniform period and bond toughness. Results are shown for three different sets of cohesive model parameters, corresponding to varying toughness and maximum cohesive stress.

The case of discontinuous pads, with an even period showed slight non-idealities. This response is not fully understood at this time, but may be a manifestation of a large-scale bridging phenomenon, or due to slight numerical error.

The simulations of discontinuous bonds of uneven period, shown in figure 14, demonstrated a pronounced non-ideal behavior. Significant load drops were observed and a rounded transition from the initial loading to the onset of fracture. The large gaps between the groups of pads is the primary source for this. In addition slight variations in the cohesive zone properties can result in significant variations in the load-deflection response, as shown in figure 14. Cohesive zone models A', D and E, varied in the toughness and peak stress in the cohesive zone model. These results indicate that even if a perfectly uniform bond quality was obtained, patterning would still result in a non-ideal load displacement response using the test method employed here.

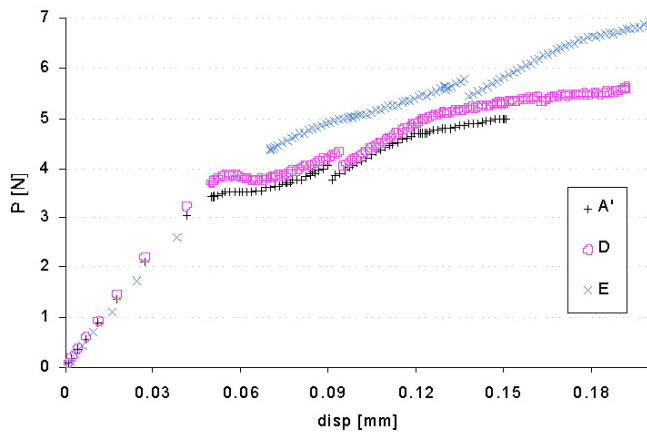


Fig. 14. Simulated load displacement response of discontinuous bond pads with uneven period. Results are shown for three cohesive models.

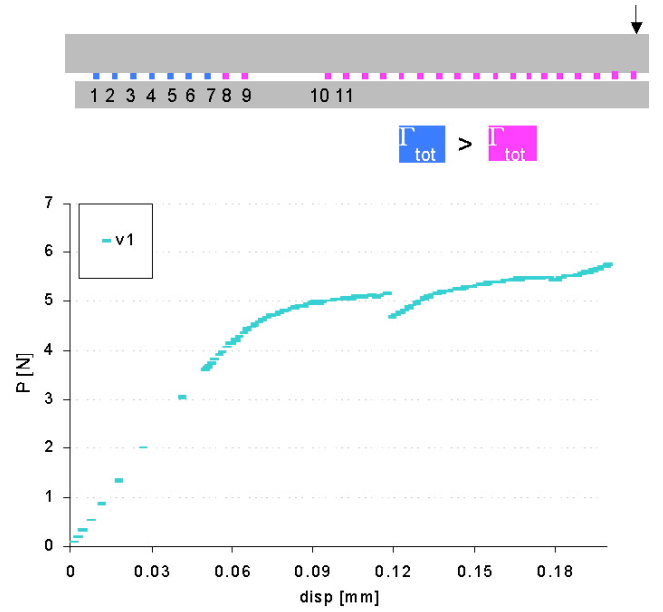


Fig. 15. Simulated load displacement response of discontinuous bond pads with uneven period for the cases in which the toughness of the bond pads nearest the starter notch was higher than the subsequent pads.

Simulations were also conducted for cases in which the toughness was varied between pads and groups of pads. Figure 15 shows the simulations for a case where the toughness of the pads in the region nearest the starter notch was higher than the pads further away. This tends to produce a somewhat flatter load-displacement response than for the case of uniform toughness.

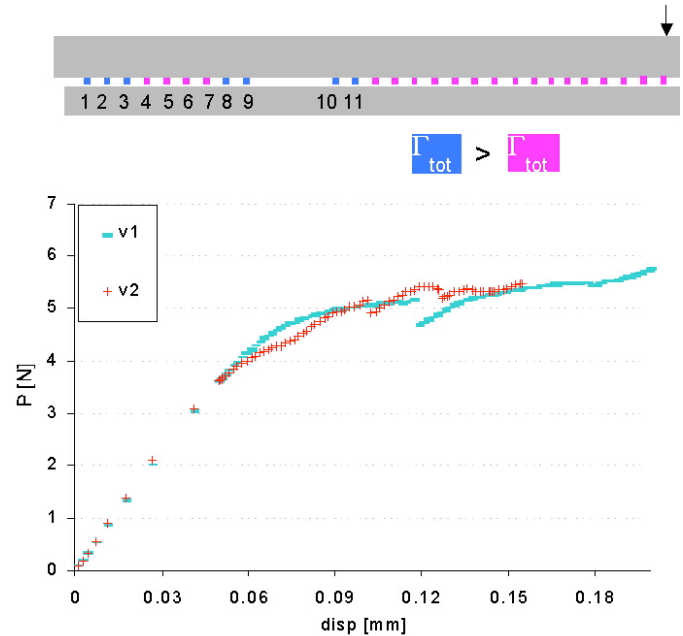


Fig. 16. Simulated load displacement response of discontinuous bond pads with uneven period for the cases in which the toughness of the bond pads varied.

Figure 16 shows results from a simulation, overlaid on that of figure 15, in which tougher and less tough pads were

intermingled with each other, resulting in yet a different predicted load-displacement response. Of particular interest in this case is the observation that the bond pads did not fail in sequence with position, weaker pads would tend to fail first, leaving one or more tougher pads left bridging between the wafers in their wake. This has the implication that the specimen compliance, or observations of crack opening displacement are not a good means of monitoring the progress of the crack tip.

The simulation results shown in figures 14-16 are qualitatively similar to the experimental results shown in figure 4. The simulations were limited to a small range of toughness values, due to convergence problems if the toughness was varied by more than 50% from one pad to the next. Notwithstanding these limitations, the results support the view that the experimentally observed variation in bond toughness (as indicated by the extent of ductility) and the experimental load deflection curves are most likely the result of variations in bond toughness across the test specimens and across the wafers combined with the patterning of the gold.

## V DISCUSSION

The modeling has provided insight regarding the variation in thermocompression wafer bond quality and the steps that will need to be taken to address it if wafer-level thermocompression bonding is to become a viable commercial process for microelectronics and MEMS fabrication and packaging. The primary source of bond quality variation is likely to be due to patterning of the gold on the wafers. For any practical application patterning is unavoidable. However, it is likely that some patterns are more or less detrimental to the ability to create a more uniform pressure distribution over the wafer surfaces to be bonded. The finite element model for the applied pressure distribution presented here provides a simple tool by which potential gold patterns can be evaluated by this metric.

Work being conducted on direct bonding of silicon wafers indicates that flatness variations in the wafers due to the cutting of the wafers from the silicon boule and the subsequent chemical-mechanical polishing (CMP) may also play a key role in thermocompression bonding [11,12]. These effects must also be taken into account in future modeling. Furthermore, it would be desirable to use a more realistic constitutive behavior for the gold in the model, and future work should include efforts to perform micro-mechanical tests on micro-fabricated gold specimens in order to determine its stress-strain response.

The cohesive zone modeling produced simulation results that were in qualitative agreement with the experimental observations. This indicates that the non-uniform patterning of the gold on the wafer bond line, combined with toughness variations between bond pads, can lead to a highly non-uniform load-displacement response.

The modeling was hampered by numerical issues, associated with the ability of the finite element solve to converge on a solution for large variations in bond toughness.

Future work must address these issues, probably by using a path following algorithm in the solver and by explicitly accounting for dynamic effects in the solution. In addition, as for the pressure-distribution modeling, it is desirable to obtain more quantitatively useful results. This requires direct measurement of the cohesive response of individual gold pads, and incorporating such data into the overall model. The same micromechanical tests proposed to examine the constitutive response of the individual gold pads under pressure loading could form the basis for conducting the reverse tests to obtain the cohesive response.

The modeling presented in this paper has provided important insight regarding the sources of variation in bond quality across wafers. In order to reduce this variation improved tooling and protocols will need to be developed. This might include the development of bonding tools that activity monitor the local pressure and adjust the applied pressure distribution in order to improve uniformity.

The mechanical test specimen used to measure the overall quality of the bonds must also be examined closely. The fact that it averages the response over a large bonded area is both an advantage and a disadvantage. The advantage is that it provides an averaged response for many pads simultaneously, which reduces the effort in testing. The disadvantage is that for device performance the failure of a single pad or a local hermetic seal can be disastrous, and an average bond toughness is not sufficient to capture these tails of the statistical distribution. In future a combination of macroscale and micro-mechanical testing is envisioned.

Finally, although this work has focused on gold thermo-compression bonding, much of the interest going forward will be on other metallic interlayers, particularly copper. This is due to the interest in creating three-dimensional interconnect structures utilizing copper as the conducting material. Copper is a harder metal than gold, and exhibits strong work hardening response as well as a tendency to oxidize. The ability to form copper thermocompression bonds reliably will require an understanding of the influence of these factors.

## VI SUMMARY AND CONCLUSIONS

This paper documents modeling of the wafer-level gold thermo-compression process. Finite element simulations were performed which provide insight regarding the sources of local pressure distribution in the process. Patterning of the gold was found to be a very significant source of such pressure variation. A cohesive zone model, in conjunction with a finite element model was used to show that patterning, in conjunction with local bond toughness variations would cause the experimentally observed non-ideal load displacement response in fracture tests.

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